

Quality Control for Theoretical Data in the Virtual Observatory: Establishing Benchmark Tests for Synthetic Spectra

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Abstract. The Virtual Observatory (VO) provides access to both, data and theory. Quality control is a general problem and the VO user needs partly some experience to judge the reliability of the VO products. As far as spectral analysis is concerned, many different areas are involved, from atomic data to stellar model-atmosphere codes.

Within the framework of the German Astrophysical Virtual Observatory (GAVO) project, the service *TheoSSA* is developed. It allows the VO user an easy access to synthetic spectral energy distributions (SEDs). We discuss quality control problems and the reliability of SEDs provided by *TheoSSA*.

1. Quality Control for Theoretical Data?

The question how to introduce quality control for theoretical data is a delicate issue. Concerning e.g. atomic data like oscillator strengths of line transitions, a comparison with observations will prove their reliability. Different algorithms for their calculation and parameter regimes for their validity can easily be evaluated.

If complex numerical simulations like model-atmosphere calculations are in focus, both, the code's level of sophistication (incl. programmed formulae, etc., cf. Mihalas 1991, 2003; Rauch 2008) and the atomic-data input contribute to the "quality" of the code's products – e.g. SEDs.

The VO provides now a platform where such SEDs of different codes can be compared to "cross check" the codes - data bases like the Tübingen Model-Atom Database *TMAD* (Sect. 5) provide model atoms that can be used by every code simply by using an appropriate adapter.

A different kind of quality control is necessary if access to SEDs is provided via a WWW interface. In case of the Tübingen NLTE Model-Atmosphere Package (*TMAP*, Sect. 2), this is done by *TheoSSA* (Sect. 3) and *TMAW* (Sect. 4). Since *TMAW* is intentionally restricted in the number of considered elements and in their model-atom representation, deviations from the most elaborated *TMAP* models that consider more elements, atomic levels, line transitions, etc. may occur. In such a case, it appears mandatory that the VO user finds reliable information about the SEDs accuracy in different wavelength ranges.

2. A Model-Atmosphere Code: *TMAP*

As an example, we use our *TMAP*¹ (Werner et al. 2003; Rauch & Deetjen 2003) that was created in the 1980s and is continuously developed since then. With *TMAP*, model atmospheres for hot, compact objects like e.g. central stars of planetary nebulae, PG 1159 stars, white dwarfs in novae, and even neutron stars can be calculated. Effective temperatures of $20\,000\,\text{K} \lesssim T_{\text{eff}} \lesssim 15\,000\,000\,\text{K}$ and surface gravities of $4 \lesssim \log g \lesssim 15$ can be chosen and elements from hydrogen to nickel (Rauch 2003; Rauch et al. 2008, 2010) can be included into the calculations. *TMAP* considers hydrostatic and radiative equilibrium, plane-parallel or spherical geometry, about 1500 atomic levels treated in NLTE, about 4000 lines from the elements H - K, and presently 200 millions of lines (Kurucz 2009) of Ca - Ni (iron-group elements).

3. SED Access: *TheoSSA*

At the end of the last century, we started to provide SEDs of hot, compact stars via our institute's WWW page. These were then used e.g. as ionizing spectra in photoionization models of planetary nebulae because the previously used blackbody fluxes are only a poor representation of a stellar spectrum. Their flux maximum is generally located at lower energies and their peak intensity is about a factor of three lower (Ringat 2012, her Fig. 1).

Within a Tübingen *GAVO* project, the registered *VO* service *TheoSSA*² was created. It is a data base to retrieve SEDs of both pre-calculated model-atmosphere grids and individual models. It is presently based on *TMAP* models but in general prepared to hold SEDs of any model-atmosphere code. SEDs that are calculated via *TMAW* (Sect. 4) are automatically ingested into *TheoSSA*. These are identified in *TheoSSA* by the entry "DataID.Creator=TMAW" in the respective meta data.

4. Individual SEDs on Demand: *TMAW*

In case that *TheoSSA* contains no SED close enough to the requested parameter values, the *VO* user is directed to *TMAW*³. This WWW interface allows to calculate *TMAP* models without profound knowledge of the code in the background. In order to keep the calculation time at a reasonable level, *TMAW*, in contrast to *TMAP*, considers only opacities of H, He, C, N, and O and uses standard model atoms that are provided by *TMAD*. These may be smaller than the detailed model atoms that are used for highly elaborated, "final" models in individual spectral analyses.

TMAW accepts also requests for model grids (in T_{eff} and $\log g$). Up to 150 models are calculated on the PC cluster of the Institute for Astronomy and Astrophysics in Tübingen. For more extended grids, *TMAW* employs the compute resources of AstroGrid-D⁴.

¹<http://astro.uni-tuebingen.de/~TMAP>

²<http://dc.g-vo.org/theossa>

³<http://astro.uni-tuebingen.de/~TMAW>

⁴<http://www.gac-grid.net>

5. A Model-Atom Data Base: *TMAD*

*TMAD*⁵ provides ready-to-use model atoms (in *TMAP* format) including level energies and radiative and collisional transition data. These are continuously updated for the most recent atomic data. Presently, it includes the elements H, He, C, N, O, F, Ne, Na, Mg, Si, S, Ar, and Ca. Complete model atoms are available for model-atmosphere and SED calculations. The latter include fine-structure splitting.

With suitable adapters, any other model-atmosphere codes can benefit from the data provided by *TMAD*.

6. A Benchmark Test: The Case of AA Doradus

The initial aim of *TheoSSA* and *TMAW* was to provide easy access to synthetic stellar fluxes for the PNe community, which was interested in realistic stellar ionizing fluxes for their PN models (Sect. 3).

It turned out rather quickly, that other groups were interested in X-ray, optical, and infrared fluxes as well. Both, *TheoSSA* and *TMAW*, were then extended for this purpose. While the accuracy in ionizing fluxes is better than 10 % compared to *TMAP* calculations with the most detailed model atoms (Ringat 2012), the precision in the optical is limited due to the smaller, standard model atoms that are used in the *TMAW* model-atmosphere calculations. The objective was here to perform preliminary spectral analyses with *TMAW* SEDs and to be better than 20 % in T_{eff} , $\log g$, and abundance determinations.

A recent spectral analysis of the sdOB primary of the binary AA Dor (Klepp & Rauch 2011) which is based on optical spectra and highly elaborated model atmospheres, that considered opacities of the elements H, He, C, N, O, Mg, Si, P, S, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, and Ni, provides an ideal test case.

Therefore, analogously to Klepp & Rauch (2011), we calculated the same model-atmosphere grid with $T_{\text{eff}} = 39\,500 - 43\,500$ K ($\Delta T_{\text{eff}} = 250$ K) and $\log g = 5.30 - 5.60$ ($\Delta \log g = 0.01$) but with the standard *TMAW* procedure, i.e. only the elements H, He, C, N, and O are considered with the standard *TMAD* model atoms (Sect. 5).

We performed a χ^2 test (for further details, see Ringat 2012), and determined $T_{\text{eff}} = 41\,150$ K and $\log g = 5.43$ while Klepp & Rauch (2011) found $T_{\text{eff}} = 40\,600$ K and $\log g = 5.46$. The deviations are only about 1 % in T_{eff} and 7 % in $\log g$. The example of AA Dor shows clearly, that *TMAW* models are already well suited for spectral analysis of optical spectra.

Further improvements of *TMAW* are currently introduced, e.g. line-formation calculations with detailed model atoms. In the near future, we will extend the considered elements to Ne, Mg, and the so-called iron-group elements (Ca-Ni).

⁵<http://astro.uni-tuebingen.de/~TMAD>

7. Summary

The *VO* constitutes an ideal environment not only to find theoretical data and simulations but also to compare them – or, in other words, to perform quality control in a broader sense. The *VO* user might encounter problems to evaluate the results of a *VO* query. Thus, it is a challenge for theory groups to intensify comparative studies (cf. Rauch 2012a).

In case of e.g. stellar model atmospheres and SEDs, a variety of LTE, NLTE, static, and expanding atmosphere codes is available and used for spectral analysis. Their validity ranges are overlapping (Rauch 2012b), allowing to cross check them in detail.

The *TheoSSA* (Theoretical Stellar Spectra Access) service is designed to provide SEDs of any kind in a *VO*-compliant form. Its efficiency is strongly increasing if more different model-atmosphere groups provide their SEDs with a proper description in their respective meta data.

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